

2015

1. Sobolev OV, **Afonine PV**, Adams PD, Urzhumtsev A. (2015). "Programming new geometry restraints: parallelity of atomic groups". *J Appl Crystallogr.* 48(Pt 4):1130-1141.
2. Urzhumtsev A, **Afonine PV**, Van Benschoten AH, Fraser JS, Adams PD. (2015). "From deep TLS validation to ensembles of atomic models built from elemental motions". *Acta Crystallogr D Biol Crystallogr.* 71(Pt 8):1668-83.
3. Van Benschoten AH, **Afonine PV**, Terwilliger TC, Wall ME, Jackson CJ, Sauter NK, Adams PD, Urzhumtsev A, Fraser JS. (2015). "Predicting X-ray diffuse scattering from translation-libration-screw structural ensembles". *Acta Crystallogr D Biol Crystallogr.* 71(Pt 8):1657-67.
4. Weichenberger CX, **Afonine PV**, Kantardjieff K, Rupp B. (2015). "The solvent component of macromolecular crystals". *Acta Crystallogr D Biol Crystallogr.* 71(Pt 5):1023-38.
5. **Afonine PV**, Moriarty NW, Mustyakimov M, Sobolev OV, Terwilliger TC, Turk D, Urzhumtsev A, Adams PD. (2015). "FEM: feature-enhanced map". *Acta Crystallogr D Biol Crystallogr.* 71(Pt 3):646-66.
6. **Afonine PV**, Urzhumtsev A, Adams PD. (2015). "Macromolecular crystallographic structure refinement". In Arbor, Celebrating 100 years of modern crystallography 2015, 191:a219.
7. McCullough J, Clippinger AK, Talledge N, Skowyra ML, Saunders MG, Naismith TV, Colf LA, **Afonine P**, Arthur C, Sundquist WI, Hanson PI, Frost A. (2015). "Structure and membrane remodeling activity of ESCRT-III helical polymers". *Science.* 350(6267):1548-51.

2014

1. Headd, J.J., Echols, N., **Afonine, P.V.**, Moriarty, N.W., Gildea, R.J. and Adams, P.D. (2014). *Flexible torsion-angle noncrystallographic symmetry restraints for improved macromolecular structure refinement*. *Acta Cryst. D70*, 1346-1356.
2. Echols, N., Morshed, N., **Afonine, P.V.**, McCoy, A.J., Miller, M.D., Read, R.J., Richardson, J.S., Terwilliger, T.C., Adams, P.D. (2014). *Automated identification of elemental ions in macromolecular crystal structures*. *Acta Cryst. D70*, 1104-1114.
3. Echols, N., Moriarty, N.W., Klei, H.E., **Afonine, P.V.**, Bunkóczki, G., Headd, J.J., McCoy, A.J., Oeffner, R.D., Read, R.J., Terwilliger, T.C. and Adams, P.D. (2014). *Automating crystallographic structure solution and refinement of protein-ligand complexes*. *Acta Cryst. D70*, 144-154.
4. Echols, N. and **Afonine, P.V.** (2014). *phenix.composite OMIT_map*. Computational Crystallography Newsletter. 5 (1), 1. (http://www.phenix-online.org/newsletter/CCN_2014_01.pdf).
5. Dar, Y., **Afonine, P.V.** and Adams, P.D. (2014). *Phenix tools for interpretation of BIOMT and MTRIX records of PDB files*. Computational Crystallography Newsletter. 5 (1), 1. (http://www.phenix-online.org/newsletter/CCN_2014_01.pdf), 8-11.

2013

1. **Afonine, P.V.**, Grosse-Kunstleve, R.W., Adams, P.D. & Urzhumtsev, A. (2013). *Bulk-solvent and overall scaling revisited: faster calculations, improved results*. *Acta Cryst. D69*, 625-634.
2. Terwilliger, T.C., Read, R.J., Adams, P.D., Brunger, A.T., **Afonine, P.V.** and Hung, L.W. (2013). *Model morphing and sequence assignment after molecular replacement*. *Acta Cryst. D69*, 2244-2250.
3. Nwachukwu, J.C., Southern, M.R., Kiefer, J.R., **Afonine, P.V.**, Adams, P.D., Terwilliger, T.C. and Nettles, K.W. (2013). *Improved crystallographic structures using extensive combinatorial refinement*. *Structure.* 5, 21(11), 1923-1930.
4. Baker, M.L., Hryc, C.F., Zhang, Q., Wu, W., Jakana, J., Haase-Pettingell, C., **Afonine, P.V.**, Adams, P.D., King, J.A., Jiang, W. and Chiu, W. (2013). *Validated near-atomic resolution*

- structure of bacteriophage epsilon15 derived from cryo-EM and modeling.* Proc Natl Acad Sci USA. 110(30), 12301-12306.
5. Urzhumtsev, A., **Afonine, P.V.** and Adams, P.D. (2013). *TLS from fundamentals to practice.* Crystallography Reviews, 19:4, 230-270.
 6. **Afonine, P.V.** and Adams, P.D. (2013). *Crystallographic Structure Refinement in a Nutshell.* Advancing Methods for Biomolecular Crystallography, NATO Science for Peace and Security Series A: Chemistry and Biology. Eds. Read RJ, Urzhumtsev, Lunin VY. Springer Science+Business Media Dordrecht. 211-219.
 7. Urzhumtsev, A.G., **Afonine, P.V.** and Lunin, V.Y. (2013). *Crystallographic Maps and Models at Low and at Subatomic Resolutions.* Advancing Methods for Biomolecular Crystallography, NATO Science for Peace and Security Series A: Chemistry and Biology. Eds. Read RJ, Urzhumtsev, Lunin VY. Springer Science+Business Media Dordrecht. 221-230.
 8. **Afonine, P.V.** (2013). *FEM: Feature Enhanced Maps.* Computational Crystallography Newsletter (2013). Volume 4, Part 2.
 9. **Afonine, P.V.**, Headd, J.J., Terwilliger, T.C. and Adams, P.D. (2013). *New tool: phenix.real_space_refine.* Computational Crystallography Newsletter. 4, 43–44.

2012

1. Terwilliger, T.C., Dimaio, F., Read, R.J., Baker, D., Bunkóczki, G., Adams, P.D., Grosse-Kunstleve, R.W., **Afonine, P.V.** & Echols, N. (2012 Mar 15). *phenix.mr_rosetta: molecular replacement and model rebuilding with Phenix and Rosetta.* J. Struct Funct Genomics.
2. Echols N., Grosse-Kunstleve, R.W., **Afonine, P.V.**, Bunkóczki, G., Chen, V.B., Headd, J.J., McCoy, A.J., Moriarty, N.W., Read, R.J., Richardson, D.C., Richardson, J.S., Terwilliger, T.C. & Adams, P.D. (2012). *Graphical tools for macromolecular crystallography in PHENIX.* J. Appl. Cryst. (2012). 45, 581-586.
3. Headd, J.J., Echols, N., **Afonine, P.V.**, Grosse-Kunstleve, R.W., Chen, V.B., Moriarty, N.W., Richardson, D.C., Richardson, J.S. & Adams, P.D. (2012). *Use of knowledge-based restraints in phenix.refine to improve macromolecular refinement at low resolution.* Acta Cryst. D68, 381-390.
4. **Afonine, P.V.**, Grosse-Kunstleve, R.W., Echols, N., Headd, J.J., Moriarty, N.W., Mustyakimov, M., Terwilliger, T.C., Urzhumtsev, A., Zwart, P.H. & Adams, P.D. (2012). *Towards automated crystallographic structure refinement with phenix.refine.* Acta Cryst. (2012). D68, 352-367.
5. **Afonine, P.V.** & Adams, P.D. (2012). *On contribution of hydrogen atoms to X-ray scattering.* Computational Crystallography Newsletter. 3, 18–21.
6. Terwilliger, T.C., Read, R.J., Adams, P.D., Brunger, A.T., Afonine, P.V., Grosse-Kunstleve, R.W. & Hung, L.-W. (2012). *Improved crystallographic models through iterated local density-guided model deformation and reciprocal-space refinement.* Acta Cryst. D68, 861-870.
7. Burnley, B.T., **Afonine, P.V.**, Adams, P.D & Gros, P. (2012). Modelling dynamics in protein crystal structures by ensemble refinement. elife., 1:e00311. doi: 10.7554/eLife.00311. Epub 2012 Dec 18.

2011

1. Urzhumtsev, A., **Afonine, P.V.** & Adams, P.D. (2011). *TLS for dummies.* Computational Crystallography Newsletter. 2, 42-84.
2. **Afonine, P.V.**, Echols, N., Grosse-Kunstleve, R.W., Moriarty, N.W. & Adams, P.D. (2011). *Improved target weight optimization in phenix.refine.* Computational Crystallography Newsletter. 2, 99–103.
3. Adams, P.D., **Afonine, P.V.**, Bunkóczki, G., Chen, V.B., Echols, N., Headd, J.J., Hung, L.W., Jain, S., Kapral, G.J., Grosse-Kunstleve, R.W., McCoy, A.J., Moriarty, N.W., Oeffner, R.D., Read, R.J.,

Richardson, D.C., Richardson, J.S., Terwilliger, T.C. & Zwart, P.H. (2011). *The Phenix software for automated determination of macromolecular structures*. Methods. **55**(1), 94-106.

2010

1. Adams, P.D., **Afonine, P.V.**, Bunkoczi, G., Chen, V.B., Davis, I.W., Echols, N., Headd, J.J., Hung, L.-W., Kapral, G.J., Grosse-Kunstleve, R.W., McCoy, A.J., Moriarty, N.W., Oeffner, R., Read, R.J., Richardson, D.C., Richardson, J.S., Terwilliger, T.C. & Zwart, P.H. (2010). *PHENIX: a comprehensive Python-based system for macromolecular structure solution*. Acta Cryst. D66, 213-221.
2. Tomanicek, S.J., Blakeley, M.P., Cooper, J., Chen, Y., **Afonine, P.V.** & Coates, L. (2010). *Neutron diffraction studies of a class A beta-lactamase Toho-1 E166A/R274N/R276N triple mutant*. J. Mol. Biol. Mar 5;396(4):1070-80.
3. Kohn, J.E., **Afonine, P.V.**, Ruscio, J.Z., Adams, P.D. & Head-Gordon, T. (2010). *Evidence of Functional Protein Dynamics from X-Ray Crystallographic Ensembles*. PLoS Computational Biology. 6(8).
4. **Afonine, P.V.**, Grosse-Kunstleve, R.W., Chen, V.B., Headd, J.J., Moriarty, N.W., Richardson, J.S., Richardson, D.C., Urzhumtsev, A., Zwart, P.H. & Adams, P.D. (2010). *phenix.model_vs_data: a high-level tool for the calculation of crystallographic model and data statistics*. J. Appl. Crystallogr. 43, 669-676.
5. Czerwinski, A., Valenzuela, F., **Afonine, P.**, Dauter, M. & Dauter, Z. (2010). *N-[2-(3,5-Difluorophenyl)acetyl]-*S*-alanyl-*S*-phenylglycine tert-butyl ester (DAPT): an inhibitor of [gamma]-secretase, revealing fine electronic and hydrogen-bonding features*. Acta Cryst. C66, o585-o588.
6. **Afonine, P.V.**, Mustyakimov, M., Grosse-Kunstleve, R.W., Moriarty, N.W., Langan, P. & Adams, P.D. (2010). *Joint X-ray and neutron refinement with phenix.refine*. Acta Cryst. D66, 1153-1163.
7. Bruning, J.B., Parent, A.A., Gil, G., Zhao, M., Nowak, J., Pace, M.C., Smith, C.L., **Afonine, P.V.**, Adams, P.D., Katzenellenbogen, J.A. & Nettles, K.W. (2010). *Coupling of receptor conformation and ligand orientation determine graded activity*. Nat Chem Biol. Nov;6(11):837-43.
8. **Afonine, P.V.**, Urzhumtsev, A., Grosse-Kunstleve, R.W. & Adams, P.D. (2010). *Atomic Displacement Parameters (ADPs), their parameterization and refinement in PHENIX*. Computational Crystallography Newsletter. 1, 24-31.

2009

1. **Afonine, P.V.**, Grosse-Kunstleve, R.W., Urzhumtsev & A., Adams, P.D. (2009). *Automatic multiple-zone rigid-body refinement with a large convergence radius*. J. Appl. 42, 607-615.
2. Urzhumtseva, L., **Afonine, P.V.**, Adams, P.D. & Urzhumtsev, A. (2009). *Crystallographic model quality at a glance*. Acta Cryst. D65, 297-300.
3. Urzhumtsev, A., **Afonine, P.V.** & Adams P.D. (2009). *On the use of logarithmic scales for analysis of diffraction data*. Acta Cryst. D65, 1283-1291.
4. Praznikar, J., **Afonine, P.V.**, Guncar, G., Adams, P.D. & Turk, D. (2009). *Averaged kick maps: less noise, more signal... and probably less bias*. Acta Cryst. D65, 921-931.
5. Adams, P.D., **Afonine, P.V.**, Grosse-Kunstleve, R.W., Read, R.J., Richardson, J.S., Richardson, D.C. & Terwilliger T.C. (2009). *Recent developments in phasing and structure refinement for macromolecular crystallography*. Current Opinion in Structural Biology. 19, 566-572.

6. Adams, P.D., Mustyakimov, M., **Afonine, P.V.** & Langan, P. (2009). *Generalized X-ray and neutron crystallographic analysis: more accurate and complete structures for biological macromolecules*. Acta Cryst. D65, 567-573.
7. Terwilliger, T.C., Adams, P.D., Read, R.J., McCoy, A.J., Moriarty, N.W., Grosse-Kunstleve, R.W., **Afonine, P.V.**, Zwart, P.H., & Hung, L.W. (2009). *Decision-making in structure solution using Bayesian estimates of map quality: the PHENIX AutoSol wizard*. Acta Cryst. D65, 582-601.

2008

1. M. Blakeley, F. Ruiz, R. Cachau, I. Hazemann, F. Meilleur, A. Mitschler, S. Ginell, **P. Afonine**, O. Ventura, A. Cousido, M. Haertlein, A. Joachimiak, D. Myles & A. Podjarny. *Quantum model of catalysis based on a mobile proton revealed by subatomic x ray and neutron diffraction studies of h-aldose reductase*. (2008). PNAS. 105, 1844-1848.
2. Terwilliger TC, Grosse-Kunstleve RW, **Afonine PV**, Moriarty NW, Zwart P, Hung LW, Read RJ & Adams PD. *Iterative model-building, structure refinement, and density modification with the PHENIX AutoBuild Wizard*. (2008). Acta Cryst. D64, 61-69.
3. Terwilliger T.C., Grosse-Kunstleve RW, **Afonine PV**, Moriarty NW, Adams PD, Read RJ, Zwart P, Hung LW. (2008). *Iterative build OMIT maps: Map improvement by iterative model-building and refinement without model bias*. Acta Cryst. (2008). D64, 515-524.
4. Langan, P., Fisher, Z., Kovalevskyi, A., Mustyakimov, M., Sutcliffe Valone, A., Unkefer, C., Waltman, M.J., Coates, L., Adams, P.D., **Afonine, P.V.**, Bennett, B., Dealwis, C., Schoenborn, B.P. *Protein structures by spallation neutron crystallography*. J. Synchrotron Rad. (2008). 15, 215-218.
5. Peter H. Zwart, **Pavel V. Afonine**, Ralf W. Grosse-Kunstleve, Li-Wei Hung, Thomas R. Ioerger, Airlie J. Mccoy, Erik McKee, Nigel W. Moriarty, Randy J. Read, James C. Sacchettini, Nicholas K. Sauter, Laurent C. Storoni, Thomas C. Terwilliger And Paul D. Adams. *Automated Structure Solution with the PHENIX Suite*. Book chapter in: Structural Proteomics High-Throughput Methods Series: Methods in Molecular Biology, Vol. 426, Kobe, Bostjan; Guss, Mitchell; Huber, Thomas (Eds.). 2008, Approx. 400 p. 130 illus., 10 in color., Hardcover, ISBN: 978-1-58829-809-6.

2007

1. Terwilliger TC, Grosse-Kunstleve RW, **Afonine PV**, Adams PD, Moriarty NW, Zwart P, Read RJ, Turk D, Hung LW. *Interpretation of ensembles created by multiple iterative rebuilding of macromolecular models*. (2007). Acta Cryst. D63, 597-610.
2. **P. Afonine** & A. Urzhumtsev. (2007). *On determination of T matrix in TLS modelling*. CCP4 Newsletter on Protein Crystallograph. 45. Contribution 6.
3. Adams PD, **Afonine, PV**, Grosse-Kunstleve RW, Moriarty NW, Sauter NK, Zwart PH, Gopal K, Ioerger TR, Kanbi L, McKee E, Pai RK, Hung L-W, Radhakannan T, McCoy AJ, Read RJ, Storoni LC, Romo TD, Sacchettini JC, Terwilliger TC: *Automated structure determination with Phenix*. In Evolving Methods for Macromolecular Crystallography. Read RJ and Sussman JL, Eds., Springer, Dordrecht, The Netherlands. 2007, 101-109.
4. **Afonine PV**, Grosse-Kunstleve RW, Adams PD, Lunin VY & Urzhumtsev AG. *On macromolecular refinement at subatomic resolution with interatomic scatterers*. (2007). Acta Cryst. D63, 1194-1197.

2006

1. Lunin, V.Y., **Afonine, P.V.** & Urzhumtsev, A.G. *Statistical modeling and likelihood-based choice in macromolecular crystallography*. (2006). Mathematical Biology & Bioinformatics. v 1, No. 1, 13-20.

2. Grosse-Kunstleve RW, Zwart PH, **Afonine PV**, Ioerger TR, Adams PD. *cctbx news*. (2006). IUCr Computing Commission Newsletter. 7:92-105.

2005

1. Grosse-Kunstleve, R.W., **Afonine, P.V.**, Sauter, N.K., Adams, P.D. *cctbx news: Phil and friends*. (2005). IUCr Computing Commission Newsletter. 5:69-91.
2. Urzhumtsev, A., Lunina, N., **Afonine, P.**, Lunin, V.Y. *Some applications of dummy scatterers for phasing in X-ray macromolecular crystallography*. In : Complutational Life Science 2005, Lecture Notes in Computer Science, eds. R.Glen, K.Diederichs, O.Kohlnacher, Springer-Verlag., Heidelberg, Computational Life Science, Konstanz, 23-25 September 2005.
3. **P.V., Afonine**, R.W., Grosse-Kunstleve & P.D., Adams. *A robust bulk-solvent correction and anisotropic scaling procedure*. (2005). *Acta Cryst.* D61, 850-855.
4. **P.V., Afonine**, R.W., Grosse-Kunstleve & P.D., Adams. *The Phenix refinement framework*. (2005). CCP4 Newsletter on Protein Crystallography. 42.

2004

1. **Afonine P.V.** & Urzhumtsev, A. *On a fast and accurate calculation of structure factors at a subatomic resolution*. (2004). *Acta Cryst.*, A60, 19-32.
2. **Afonine P.V.**, Lunin, V., Muzet, N. & Urzhumtsev, A. *On the possibility of observation of valence electron density for individual bonds in proteins in conventional difference maps*. (2004). *Acta Cryst.*, D60, 260-274.
3. Grosse-Kunstleve, R.W., **Afonine, P.V.**, Adams, P.D. *cctbx news*. (2004). IUCr Computing Commission Newsletter. 4:19-36.

2003

1. **Afonine P.V.**, Lunin, V.Y. & Urzhumtsev, A.G., *MLMF program: maximum likelihood estimates for weights and target values in least-squares refinement*. *J. Appl. Cryst.* (2003). 36, 158-159.

2002

2. **Afonin, P.V.**, Fokin, A.V., Tsygannik I.N., Pletnev S.V., Duax W., Pletnev, V.Z., *Three-Dimensional Structure of the Arg32His Mutant of the Human Tumor Necrosis Factor Determined at 2.5A Resolution from X-ray Data for a Twin Crystal*. *Crystallography Reports*, Vol. 47, No. 4, (2002), pp. 629-634 (translated from Kristallographiya, Vol. 47, No. 4, 2002, pp. 685-690).
3. V.Y. Lunin, **P.V. Afonine** & A.G. Urzhumtsev. *Irremovable model errors and the likelihood based refinement*. (2002). *Acta Cryst.*, A58, 270-282.
4. **Afonine P.V.** *Atomic displacement in incomplete models caused by optimization of crystallographic criteria*. (2002). CCP4 Newsletter on Protein Crystallography. 41.
5. **Afonine P.V.**, Lunin, V.Y. & Urzhumtsev, A.G., *Search of the optimal strategy for refinement of atomic models*. (2002). CCP4 Newsletter on Protein Crystallography. 40.
6. **Afonine, P.V.**, Pichon-Pesme, V., Muzet, N., Jelsch, C., Lecomte, C. & Urzhumtsev, A. *Modeling of bond electron density*. (2002). CCP4 Newsletter on Protein Crystallography. 41.

2001

1. **Afonin P.V.**, Fokin A.V., Tsygannik I.N., Mikhailova I.Yu., Mikhaleva I.I., Onoprienko L.V., Ivanov V.T., Mareeva T.Yu., V.A. Nesmeyanov V.A., Li N., Duax W.L., Pletnev V.Z. *Crystal Structure of an anti-interleukin-2 monoclonal antibody Fab complexed with an antigenic nonapeptide*. (2001). *Protein Sci.*, 10(8), 1514-21.
2. **Afonine P.V.**, Lunin, V.Y. & Urzhumtsev, A.G. *Maximum-Likelihood Refinement of Atomic Models Using Least-Squares Criterion*. (2001). CCP4 Newsletter on Protein Crystallography, 2001, 39: pp. 52-56.

2000

1. Fokin A.V., **Afonin P.V.**, Mikhailova I.Yu, Tsygannik I.N., Mareeva T.Yu, Nesmeyanov V.A., Pangborn W., Lee N, Duax W., Cizhak E., Pletnev V.Z. *Three-dimensional structure of Fab fragment of monoclonal antibody LNKB-2 against human interleukin-2 in two crystal forms at 2.2 and 2.9A resolution..* Russian Journal of Bioorganic Chemistry, Vol. 26, No. 8, (2000), pp. 512-519. Translated from Bioorganicheskaya Khimiya, Vol. 26, No. 8, 2000, pp. 571-578.